

Phase separation in a boson-fermion mixture of Lithium atoms

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Abstract. We use a semiclassical three-fluid model to analyze the conditions for spatial phase separation in a mixture of fermionic ${}^6\text{Li}$ and a (stable) Bose-Einstein condensate of ${}^7\text{Li}$ atoms under cylindrical harmonic confinement, both at zero and finite temperature. We show that with the parameters of the Paris experiment [F. Schreck *et al.*, Phys. Rev. Lett. **87** 080403 (2001)] an increase of the boson-fermion scattering length by a factor five would be sufficient to enter the phase-separated regime. We give examples of configurations for the density profiles in phase separation and estimate that the transition should persist at temperatures typical of current experiments. For higher values of the boson-fermion coupling we also find a new phase separation between the fermions and the bosonic thermal cloud at finite temperature.

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1. Introduction

Following the achievement of Bose-Einstein condensation in alkali gases [1], a great deal of experimental effort is being devoted to trap and cool gases of fermionic isotopes of alkali atoms. The usual evaporative cooling scheme is ineffective, since the Pauli exclusion principle forbids s -wave collisions between spin-polarized fermions. This problem has been circumvented by recourse to sympathetic cooling, which relies on s -wave collisions with atoms belonging to different species, and several groups have thus reached in the Fermi cloud temperatures as low as $T = 0.2 T_F$ [2, 3, 4], T_F being the Fermi temperature. In particular, an experiment in Paris has produced a mixture of a degenerate Fermi gas and a stable Bose-Einstein condensate, made from Lithium isotopes [4].

The condensate-fermion mixture is an interesting system for the study of the effects of the interactions, since it can show spatial phase separation of the two components on increasing the value of the boson-boson and boson-fermion coupling constants [5]. This is an example of a quantum phase transition [6]. Several configurations for phase-separated clouds have been proposed in [7]. A schematic phase diagram for the trapped boson-fermion mixture at zero temperature has been given in [8], while the phases and the stability of a homogeneous boson-fermion mixture have been studied in [9]. In the experiments it might be possible to investigate the phase-separated region by exploiting optically or magnetically induced Feshbach resonances to increase the values of the boson-boson and/or the fermion-boson scattering length [10].

In this letter we have chosen the trap geometry and parameters typical of the Paris experiment and have analyzed the possible phase-separated configurations; we also indicate how various equilibrium observables are affected by phase separation.

The paper is organized as follows: in Sec. 2 we present the model which we have used and discuss its limits of applicability; Sec. 3 gives the conditions for phase separation at zero temperature and illustrates the column-density profiles corresponding to different phase-separated configurations. The results are extended to finite temperature in Sec. 4.

2. The model

We adopt a three-fluid model for a mixture of bosons and fermions at finite temperature T [11]. The model is used to evaluate the density profile of the condensate (n_c) within the Thomas-Fermi approximation and those of the fermionic (n_f) and thermal bosonic component (n_{nc}) within the Hartree-Fock approximation.

We shall assume that the number of bosons in the trap is large enough that the kinetic energy term in the Gross-Pitaevskii equation for the wave function $\psi(\mathbf{r})$ of the condensate can be neglected [12]. The density profile of the condensed atoms is

$$n_c(\mathbf{r}) = \psi^2(\mathbf{r}) = [\mu_b - V_b^{ext}(\mathbf{r}) - 2gn_{nc}(\mathbf{r}) - fn_f(\mathbf{r})]/g \quad (1)$$

for positive values of the function in the brackets and zero otherwise. Here, $g = 4\pi\hbar^2 a_{bb}/m_b$ and $f = 2\pi\hbar^2 a_{bf}/m_r$ with a_{bb} and a_{bf} the boson-boson and boson-fermion s -

wave scattering lengths and $m_r = m_b m_f / (m_b + m_f)$ with m_b and m_f the atomic masses; μ_b is the chemical potential of the bosons. The system is confined by external axially symmetric potentials

$$V_{b,f}^{ext}(\mathbf{r}) = m_{b,f} \omega_{b,f}^2 (r^2 + \lambda_{b,f}^2 z^2) / 2 \quad (2)$$

where $\omega_{b,f}$ are the frequencies and $\lambda_{b,f}$ the anisotropies of the traps.

As already proposed in early work on the confined Bose fluid [13], we treat both the thermal bosons and the fermions as ideal gases in effective potentials $V_{b,f}^{eff}(\mathbf{r})$ involving the relevant interactions. We write

$$V_b^{eff}(\mathbf{r}) = V_b^{ext}(\mathbf{r}) + 2gn_c(\mathbf{r}) + 2gn_{nc}(\mathbf{r}) + fn_f(\mathbf{r}) \quad (3)$$

and

$$V_f^{eff}(\mathbf{r}) = V_f^{ext}(\mathbf{r}) + fn_c(\mathbf{r}) + fn_{nc}(\mathbf{r}). \quad (4)$$

We are taking the fermionic component as a dilute, spin-polarized Fermi gas: the fermion-fermion interactions are then associated at leading order with p -wave scattering and are negligible at the temperatures of present interest [14]. Here and in Eq. (1), the factors 2 arise from exchange.

We may then evaluate the thermal averages by means of standard Bose-Einstein and Fermi-Dirac distributions, taking the thermal bosons to be in thermal equilibrium with the condensate at the same chemical potential and the fermions at chemical potential μ_f . In this semiclassical approximation the densities of the cold-atom clouds are

$$n_{nc,f}(\mathbf{r}) = \int \frac{d^3p}{(2\pi\hbar)^3} \left\{ \exp \left[\left(\frac{p^2}{2m_{b,f}} + V_{b,f}^{eff}(\mathbf{r}) - \mu_{b,f} \right) / k_B T \right] \mp 1 \right\}^{-1}. \quad (5)$$

The chemical potentials are determined from the total numbers of bosons and fermions.

The above model is valid for bosons when the diluteness condition $n_c a_{bb}^3 \ll 1$ holds. For the Fermi cloud in the mixed regime the condition $k_f a_{bf} \ll 1$ with $k_f = (48N_F)^{1/6} / a_{ho}$ should hold, but this is not a constraint in the regime of phase separation where the boson-fermion interaction energy drops rapidly (see below).

3. Conditions for phase separation

Phase separation is complete when the overlap between the bosonic and the fermionic density profiles vanishes. The transition to this regime depends on the confinement and on the numbers, masses and interaction strengths of the trapped fermions and bosons. In the case of equal numbers of bosons and fermions and equal trapping frequencies the condition of phase separation can be written as

$$k_f a_{bb} > \frac{3\pi}{4} \left(\frac{a_{bb}}{a_{bf}} \right)^2 \quad (6)$$

at zero temperature [8, 9].

Let us focus on the geometry and on typical values of the numbers of atoms in the Paris experiment [4] for the ^7Li - ^6Li mixture: $\omega_b = 2\pi \times 4000$ Hz, $\omega_f = 2\pi \times 3520$ Hz,

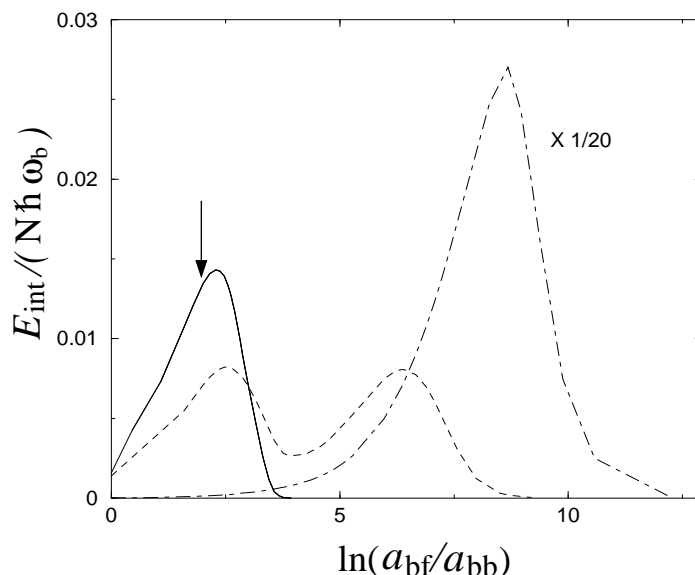


Figure 1. Boson-fermion interaction energy (in units of $N\hbar\omega_b$ with $N = 20000$ being the total number of particles), as a function of $\ln(a_{bf}/a_{bb})$. The curves are obtained for $a_{bb} = 5.1 a_0$ and equal numbers of bosons and fermions at various values of the temperature: $T = 0$ (solid line), $T = 0.2 T_F$ (dashed line) and $T = 0.6 T_F$ (dotted-dashed line, on a scale reduced by a factor 20). The arrow indicates the location of the Paris experiment.

$\lambda_b \simeq \lambda_f \simeq 1/60$, and $N_b \simeq N_f \simeq 10000$. Since the two trap frequencies are of the same order of magnitude, we can use Eq. (6) to estimate at which values of the scattering lengths the phase transition occurs. For the above experimental parameters the condition (6) becomes $\xi \equiv a_{bf}^2/a_{bb} > 7000 a_0$. Using the predicted values for the scattering lengths of the ^7Li - ^6Li mixture, that is $a_{bb} = 5.1 a_0$ and $a_{bf} = 38 a_0$ [4], we have $\xi \simeq 283 a_0$ and the gases are not as yet in the phase-separated regime. However, in a Feshbach-resonance experiment the scattering lengths could be increased. There is therefore the possibility to fulfill Eq. (6) and to enter the phase-separated regime.

Since the positions of the Feshbach resonances for a_{bf} and a_{bb} would not necessarily coincide, in order to explore the phase diagram for the boson-fermion mixture we have first of all kept a_{bb} fixed at its non-resonant value and changed a_{bf} . In this case, in order to reach phase separation it is sufficient to increase the value of the boson-fermion scattering length by a factor five, namely $a_{bf} > \tilde{a}_{bf} \simeq 200 a_0$.

To check this estimate we have evaluated the boson-fermion interaction energy

$$E_{int} = f \int d^3r [n_c(\mathbf{r}) + n_{nc}(\mathbf{r})] n_f(\mathbf{r}), \quad (7)$$

using the model described in Sec. 2. The behaviour of this quantity at $T = 0$ as a function of a_{bf}/a_{bb} , with $a_{bb} = 5.1 a_0$, is shown in Fig. 1 (solid line). Because of finite size effects the transition to the phase-separated regime shows a large crossover region and the interaction energy goes smoothly to zero when separation is complete [15].

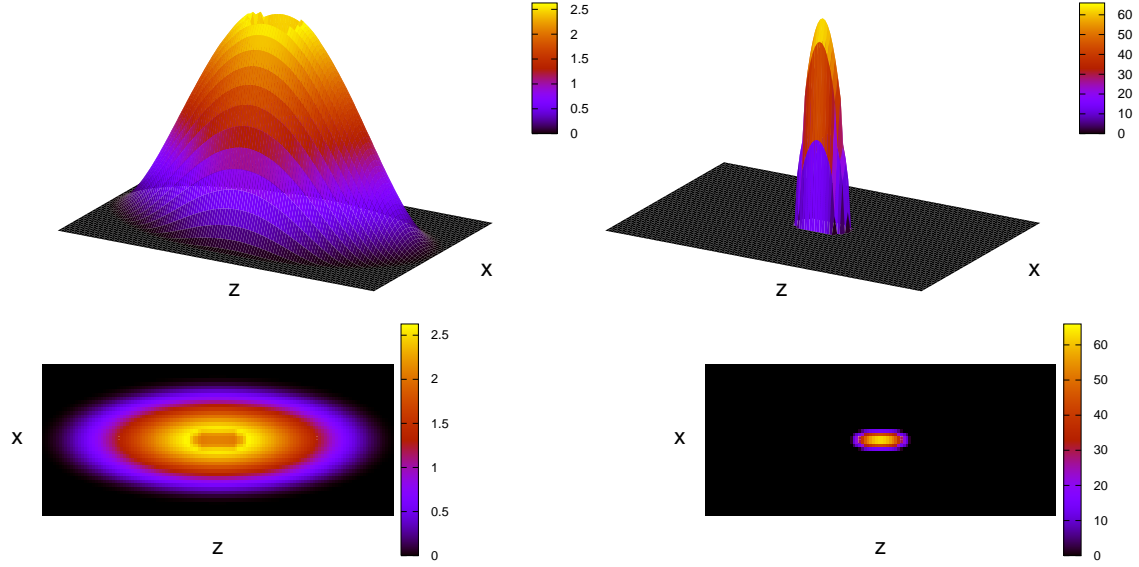


Figure 2. The symmetric configuration at the threshold of the phase-separation regime, obtained for $a_{bb} = 5.1 a_0$ and $a_{bf} = 200 a_0$. Top panels: column densities in the $\{x, z\}$ plane of the fermionic cloud (left) and of the condensate (right); bottom panels: topview images of the same profiles. The size of the figures in the $\{x, z\}$ plane is $10\mu\text{m} \times 665\mu\text{m}$.

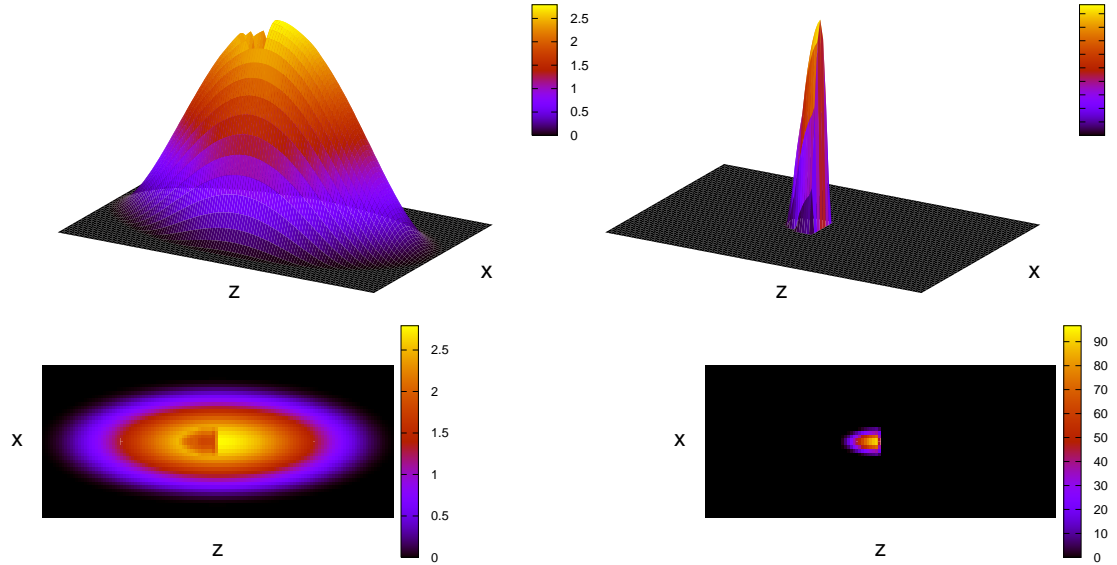


Figure 3. The fully asymmetric configuration for $a_{bb} = 5.1 a_0$ and $a_{bf} = 1000 a_0$. Top panels: column densities in the $\{x, z\}$ plane of the fermionic cloud (on the left) and of the condensate (on the right); bottom panels: topview images of the same profiles. The size of the figures in the $\{x, z\}$ plane is $10\mu\text{m} \times 665\mu\text{m}$.

For the value $a_{bf} = 38a_0$ corresponding to the current experiments (marked by the arrow in Fig. 1), the boson-fermion interaction energy is close to its maximum value. We find that the overlap between the two clouds vanishes if $a_{bf} > 200a_0$, in accord with the estimate given just above.

To make close contact with experiments we have calculated the column densities of the fermionic and condensate vapours in the phase-separated regime for various values of a_{bf} . At the threshold value we have found only one possible configuration, with a central hole in the fermionic cloud which is occupied by the condensed bosons (see Fig. 2). For this configuration there is only a quantitative difference in the value of the contrast at the center of the fermionic cloud as compared to the mixed state.

The regime of phase separation is univocally characterized by the presence of other configurations at higher values of a_{bf} . Starting from different initial conditions, for $1000a_0 < a_{bf} < 2000a_0$ we have found, in addition to a configuration which is similar to that in Fig. 2, another with a different ellipticity of the hole and a third one which is asymmetric in the axial direction (see Fig. 3). For the values of the parameters that we have used the lowest energy configuration is the first (symmetric) one. However, also the other metastable states are close in energy and could perhaps be realized in the laboratory by applying an adiabatic perturbation having the symmetry of the final state. The asymmetric state could easily be identified in the column-density pictures.

Other interesting configurations would be observed in an experiment in which both scattering lengths could be changed. On increasing a_{bb} the size of the condensate increases towards that of the fermion cloud and the hole in the latter widens, until a situation is reached in which the fermions are pushed out in the radial direction and make a ring around a cigar of bosons. Another peculiar shape is a “double sandwich” of bosons, in which two slices of condensate are separated by a central slice of fermions and surrounded by a fermionic shell. As a last remark, the energy of all these configurations depends on the values of the scattering lengths: it may thus happen that the most stable state is the asymmetric one or has other exotic shapes [16].

4. Effects of temperature

At low temperature ($T \sim 0.2T_F$) the density profiles for the various configurations are essentially the same as those found at $T = 0$, with the addition of a small bosonic thermal cloud. For values of the boson-fermion scattering length around the critical value \tilde{a}_{bf} the phase separation involves only the condensate and the fermionic cloud: the total boson-fermion interaction energy E_{int} has a minimum but does not vanish (see the dashed line in Fig. 1), since the fermionic and the bosonic thermal clouds still overlap. However, with a further increase in the scattering length, up to values of order $10^5 a_0$, the model yields full phase separation between fermions and bosons.

At higher temperature ($T \sim 0.6T_F$) we do not find phase separation between the fermionic cloud and the condensate (see the dotted-dashed line in Fig. 1). Separation between the total bosonic gas and the fermions is instead found in this model at

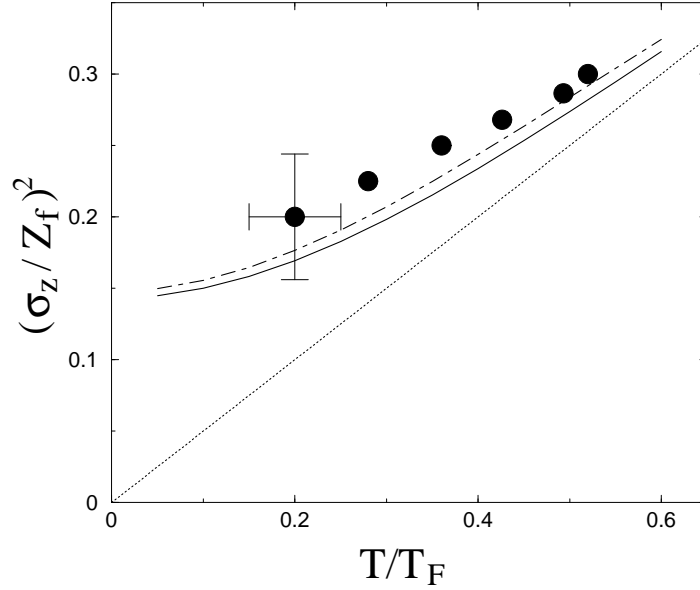


Figure 4. Variance of the axial distribution of a cloud of 10000 atoms of ${}^6\text{Li}$ taken at $x = 0$ (in units of $Z_f^2 = 2k_B T_F / m_f \omega_f^2$) against T/T_F with $T_F = (6N_f)^{1/3} \hbar \omega_f / k_B$. The experimental data (filled circles; from Ref [4] and private communication) are compared with the behaviour of the classical gas (dotted line), of the ideal Fermi gas (full line), and of the fermionic cloud interacting with its bosonic partner ($N_b = 20000$) using the values $a_{bb} = 5.1 a_0$ and $a_{bf} = 200 a_0$ (dotted-dashed line).

$a_{bf} \sim 10^5 a_0$. In this case a symmetric configuration is generated, in which the fermions are pushed outside the whole boson gas. The size of the hole in the fermionic cloud is determined by the width of the bosonic thermal cloud, making the finite-temperature transition much more evident in the column-density images than at $T = 0$ [16].

Another quantity which can be measured as a function of temperature is the width of the fermionic density profile in a given direction, *e.g.* in the z direction (see Fig. 4). While for the values of the scattering lengths in the Lithium experiment the width is predicted to be almost the same as that of the non-interacting Fermi gas [17], larger increases in width are found in some phase-separated configurations. This observable is particularly sensitive to the configurations which involve a large displacement of the fermions, such as the “double boson sandwich” [16].

In conclusion, we have examined the main observable features of spatial phase separation in gaseous mixtures of Li isotopes, with specific focus on the setup of the Paris experiments. A full account of our results will be given elsewhere [16].

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